Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 90.2 mmHg

Global applicability domain: Inside

Local applicability domain index: 4.31e-01

Confidence level: 4.24e-01

Nearest Neighbors from the Training Set

Image not found
Trichloroacetic acid
Measured: 23.8
Predicted: 2.18e-01

Image not found
1-Dodecanamine
Measured: 48300
Predicted: 1.46e-02

Image not found
1-Fluorododecane
Measured: 7050
Predicted: 1.40e-01

Image not found
Vinylidene fluoride
Measured: 1420
Predicted: 7860

Image not found
Ketene
Measured: 9410
Predicted: 1800